Neutron scattering research on organic solar cell materials

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Neutrons and energy for the future

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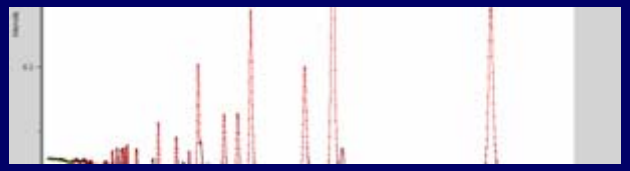
Group activities in energy storage and conversion materials

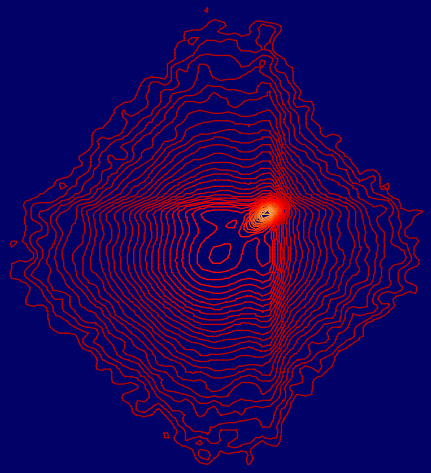
Main microscopic techniques:

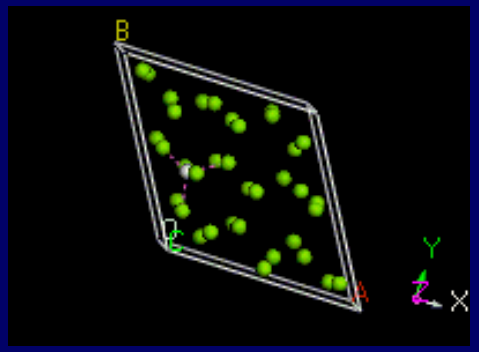
Neutron scattering

NMR

Modeling







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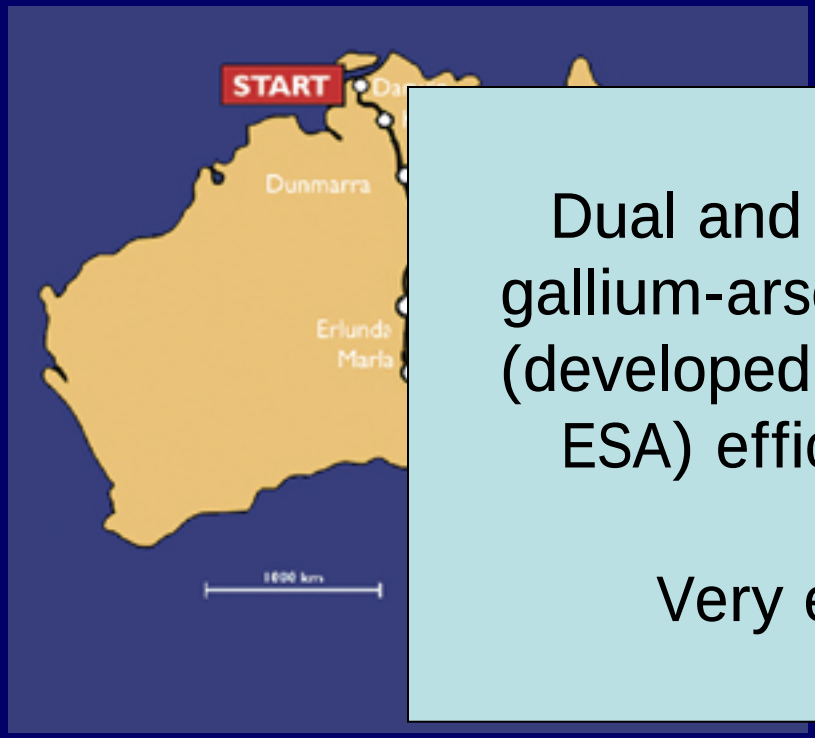
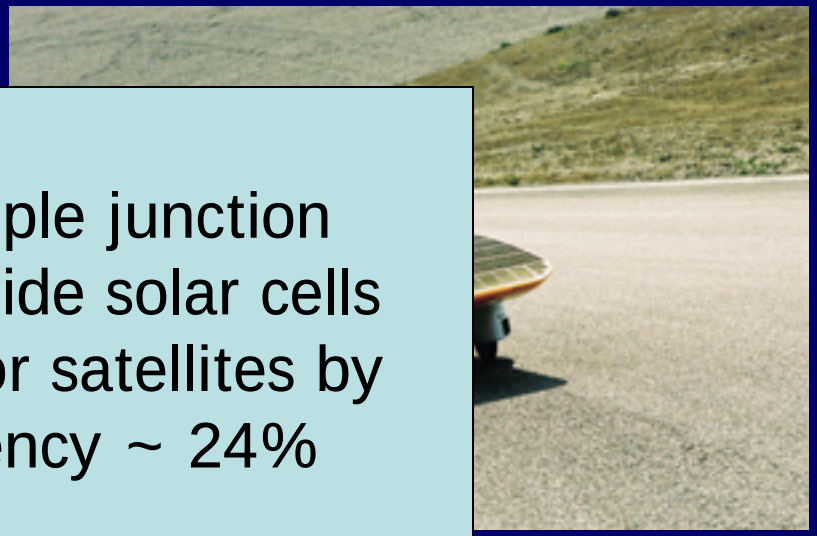
Solar energy applications

Team of Delft University wins World Solar Challenges 2001, 2003





Dual and triple junction gallium-arsenide solar cells (developed for satellites by ESA) efficiency ~ 24%

Very expensive!

ed: 175 kph
l 97 kph

Energy payback ratio =

$$\frac{\text{usable energy delivered during lifetime}}{\text{energy used for building \& running device/plant}}$$

Solar cell (monocrystalline)	5 - 7
Solar cell (thin film, organic)	15 - 20
Wind	30 – 40
D-T Fusion	(27)
Fission	~ 16
Coal:	11 - 14
Gasoline	10 – 40 ??

Organic solar cell by self-assembly?

L. Schmidt-Mende *et al.* Science 293 (2001) 1119 & 1059

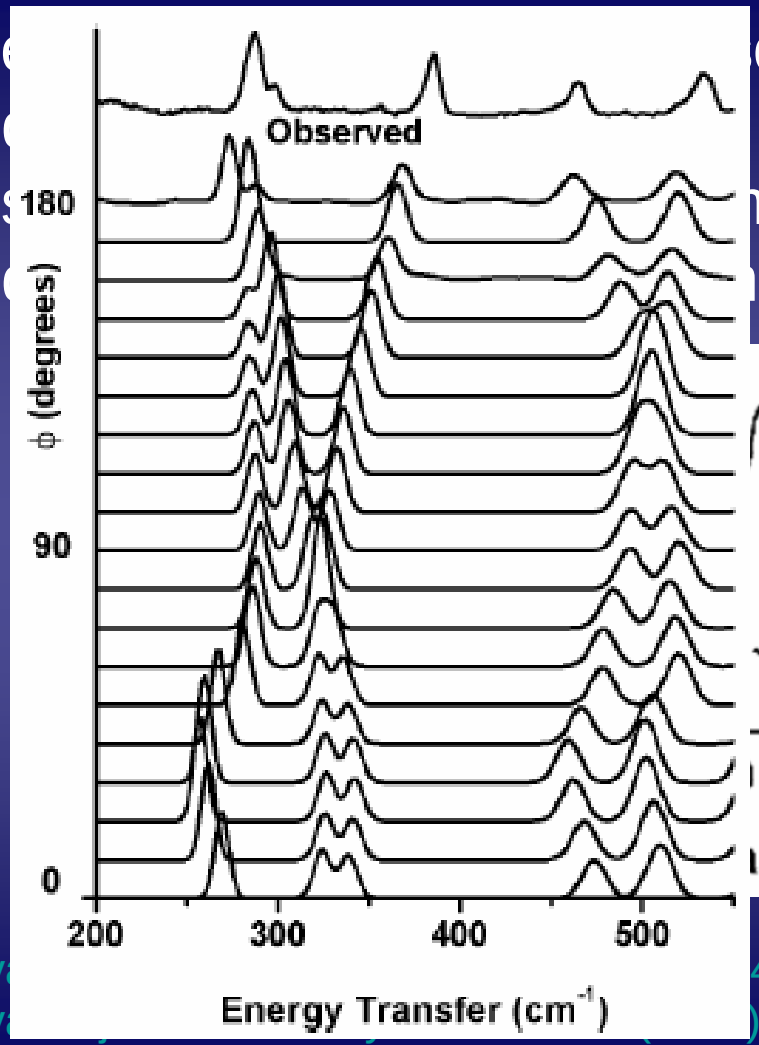
Grätzel type solar cells using organic dyes:
efficiency up to 11%

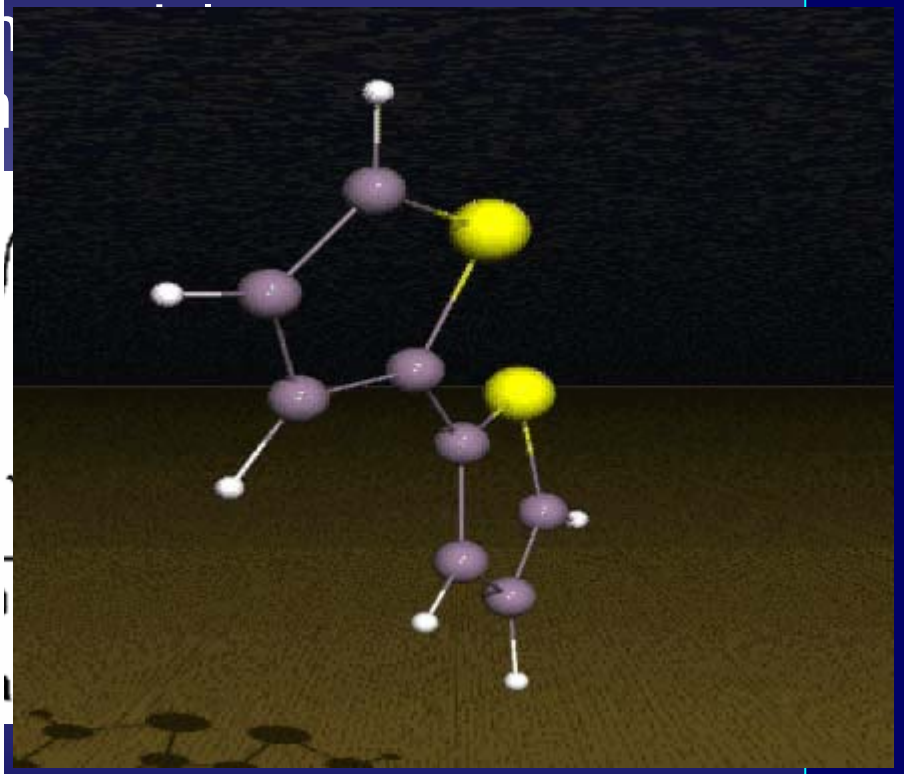
Overview: see e.g. M. Grätzel, Nature 414 (2001) 338.

Hole conducting organic dye: Polythiophene

N copy:

-
-
-





TOSCA, ISIS

L. v 496
L. v) 42.

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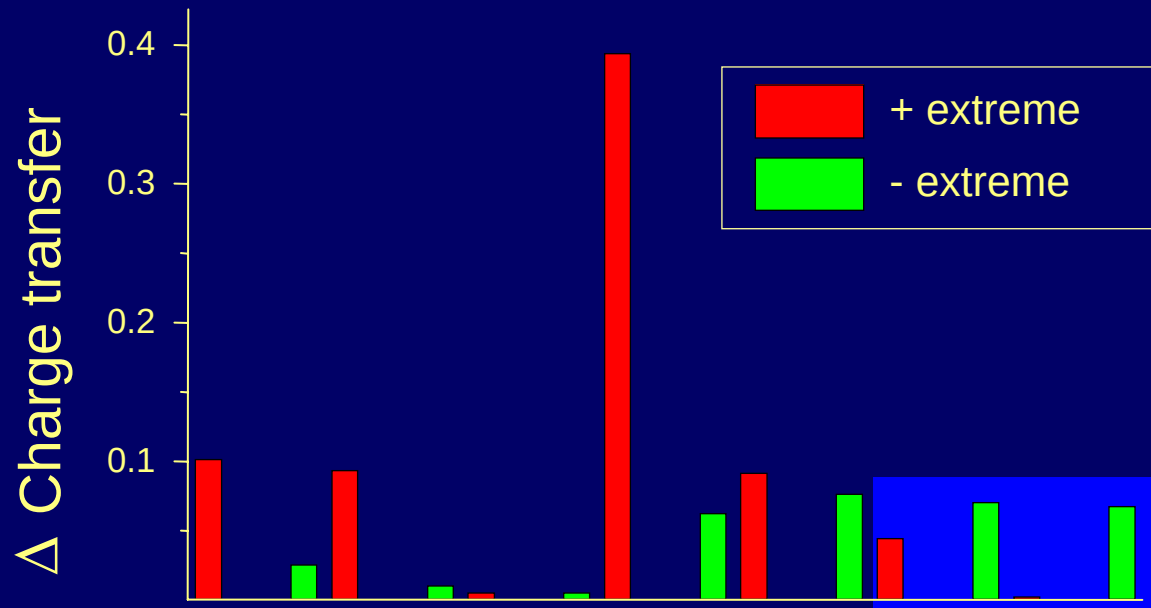
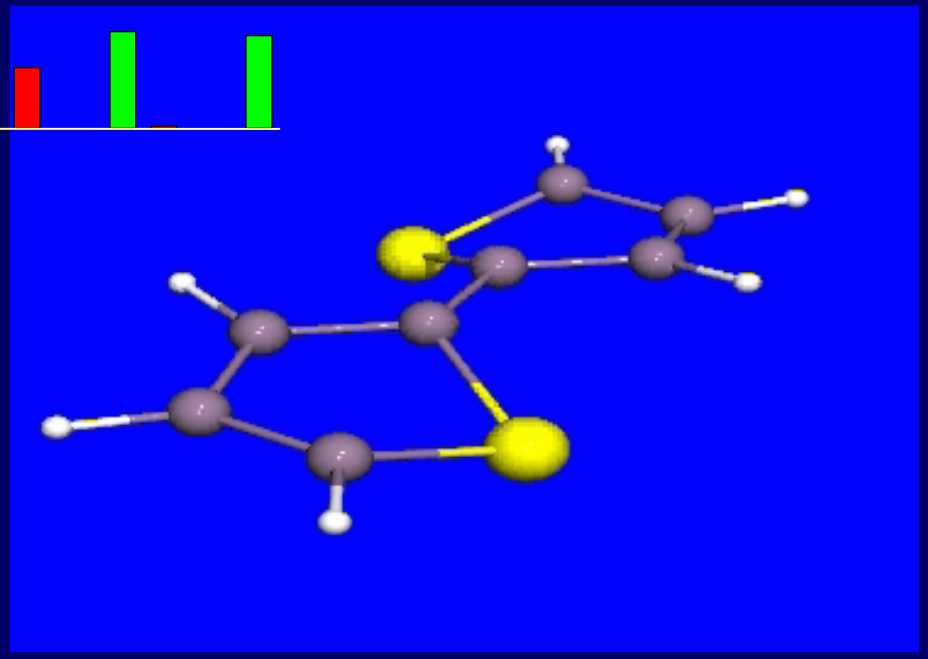


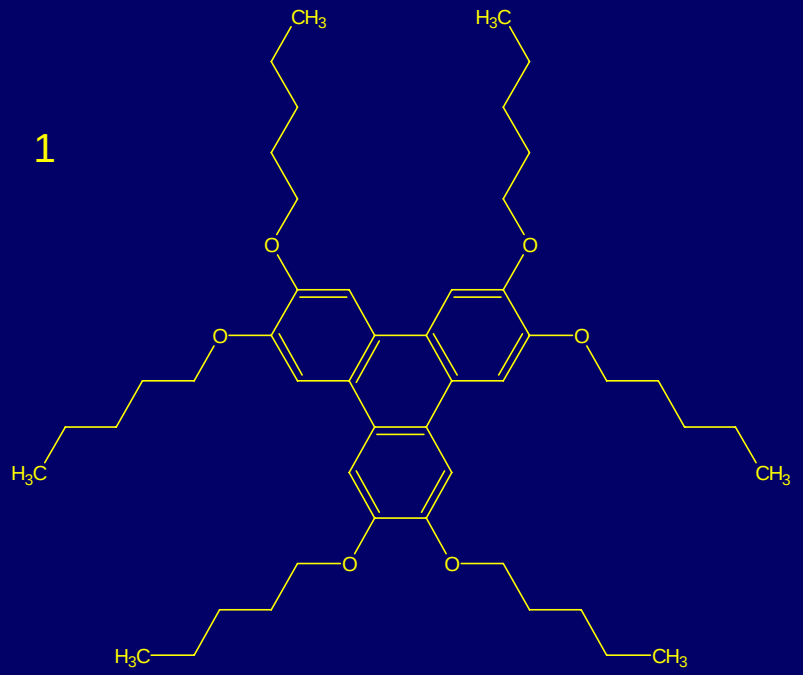


Main effect:
p ↔ s character transfer

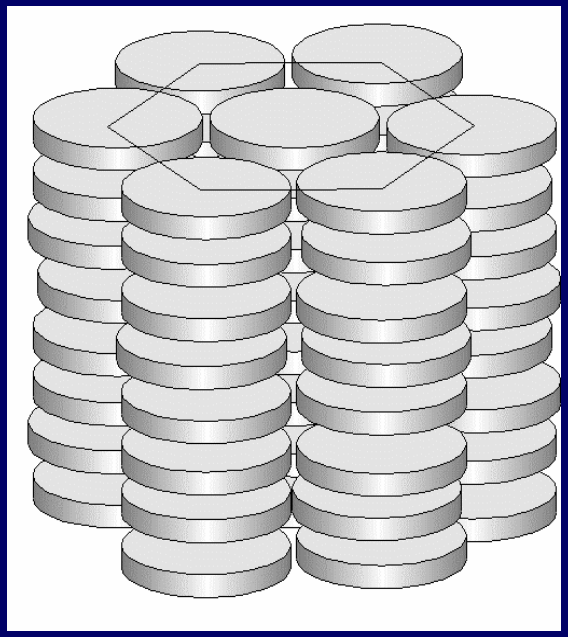
Co-continuous network of perylene electron conductor and discotic hole conductor

Model compound for discotics:
hexa-alkoxy triphenylene: HAT6

1



Liquid crystalline
Between 69 and 99 ^{o}C



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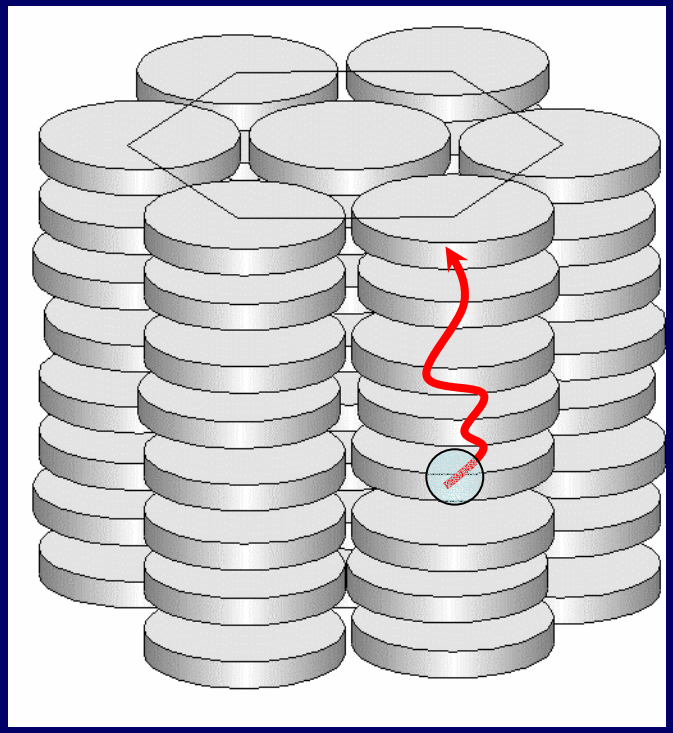
Charge transport along columns:

→ inter-disc hopping on ps timescales

→ long-range transport over ~100 nm on ~ns

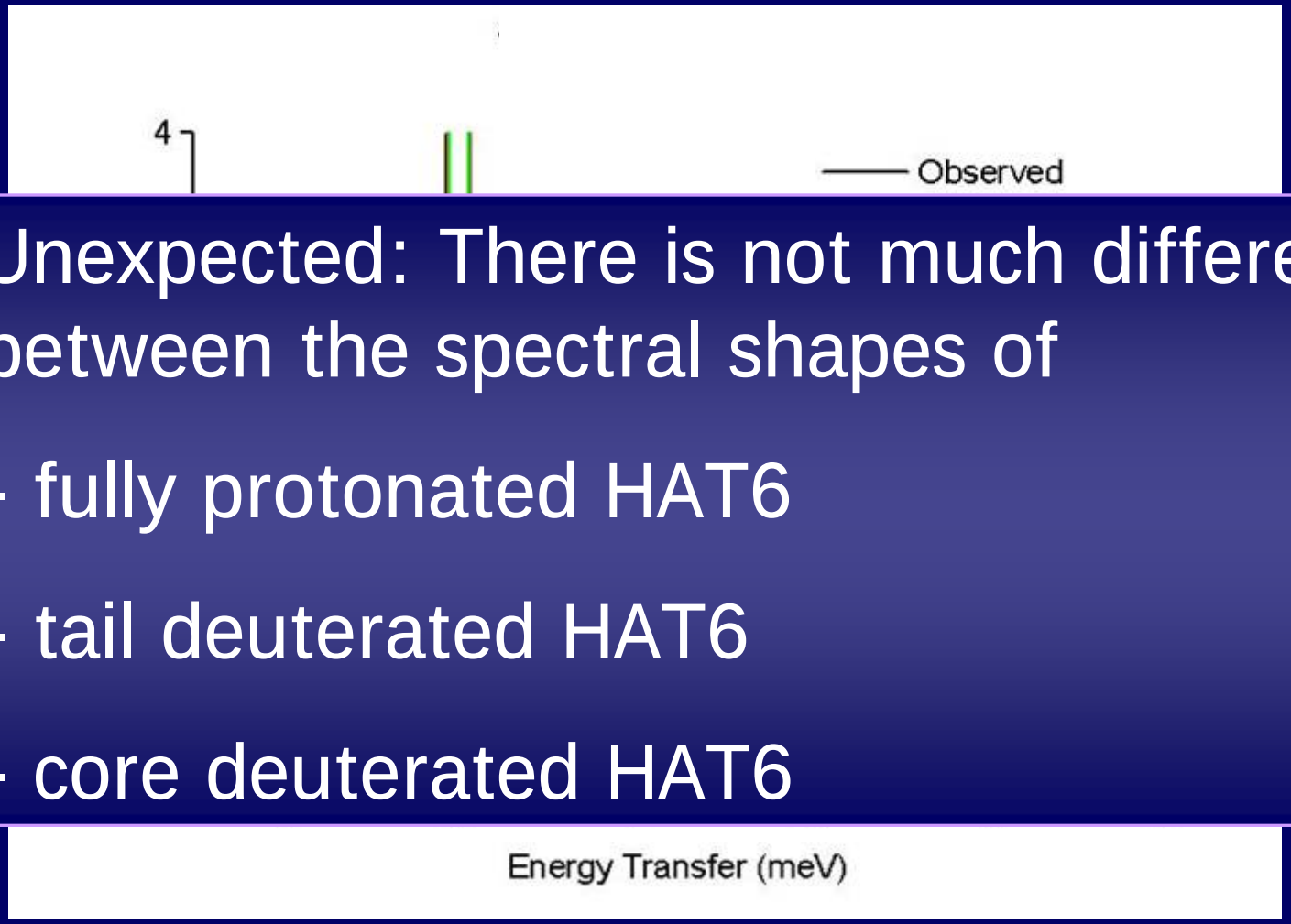


ps

Could molecular motion influence charge transfer?

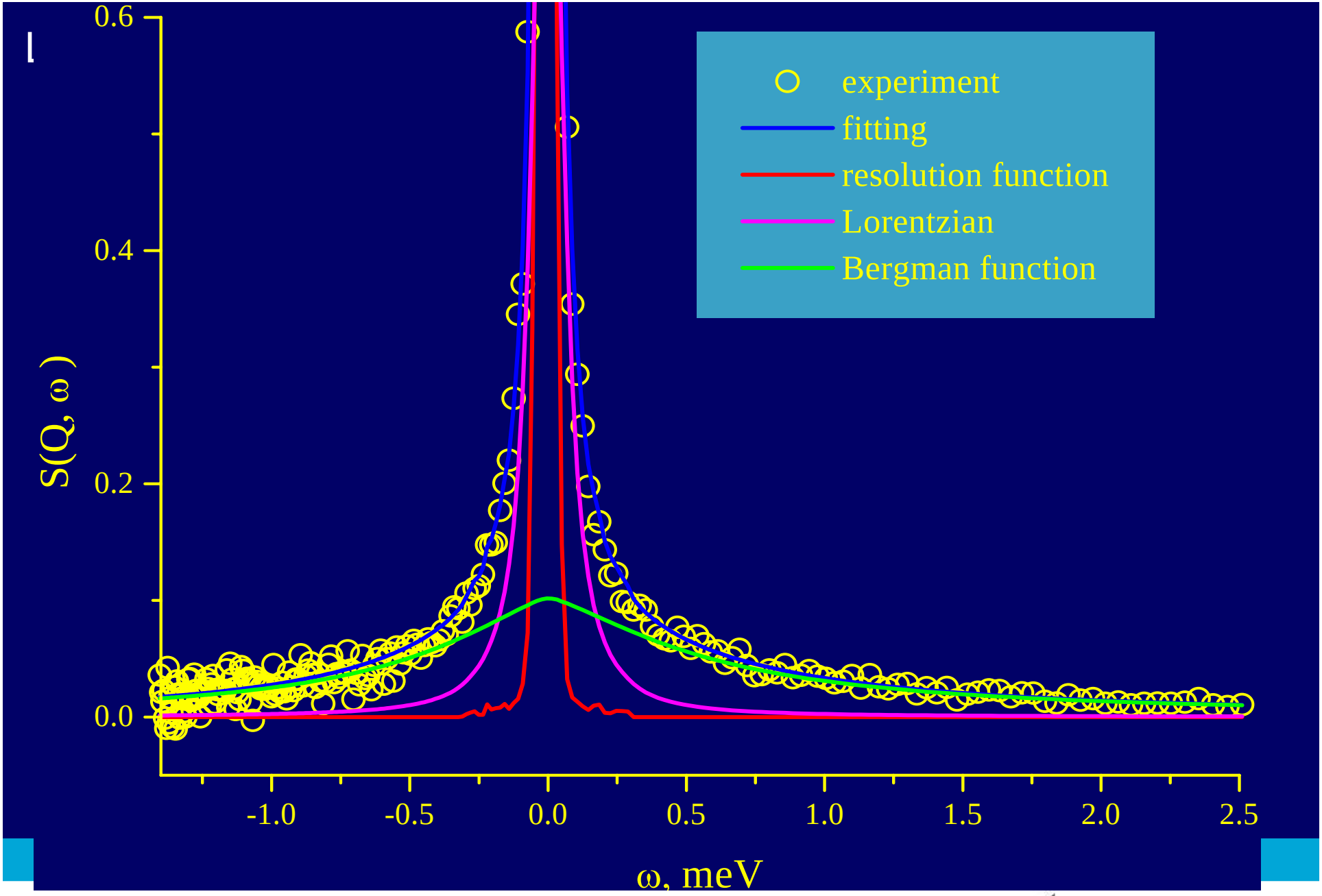
A.M. van de Craats *et al.* J. Phys. Chem. B102 (1998) 9625.

Quasi elastic neutron scattering (IN6, ILL, Grenoble)

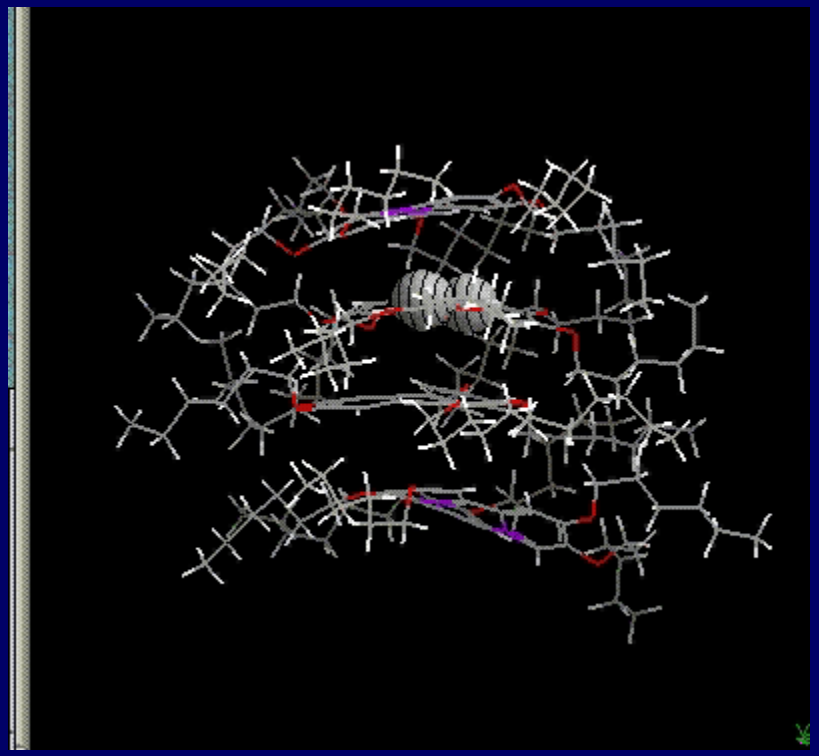


Unexpected: There is not much difference between the spectral shapes of

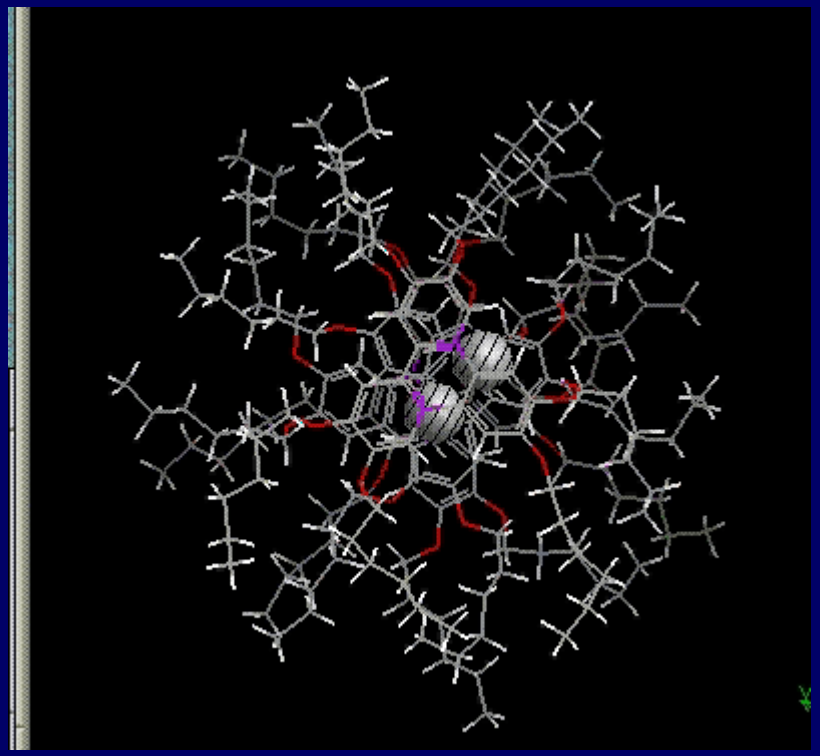
- fully protonated HAT6
- tail deuterated HAT6
- core deuterated HAT6


experiment
fitting
resolution function
Lorentzian
Bergman function
S(Q, ω)
0.6
0.4
0.2
0.0
-1.0
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
ω, meV

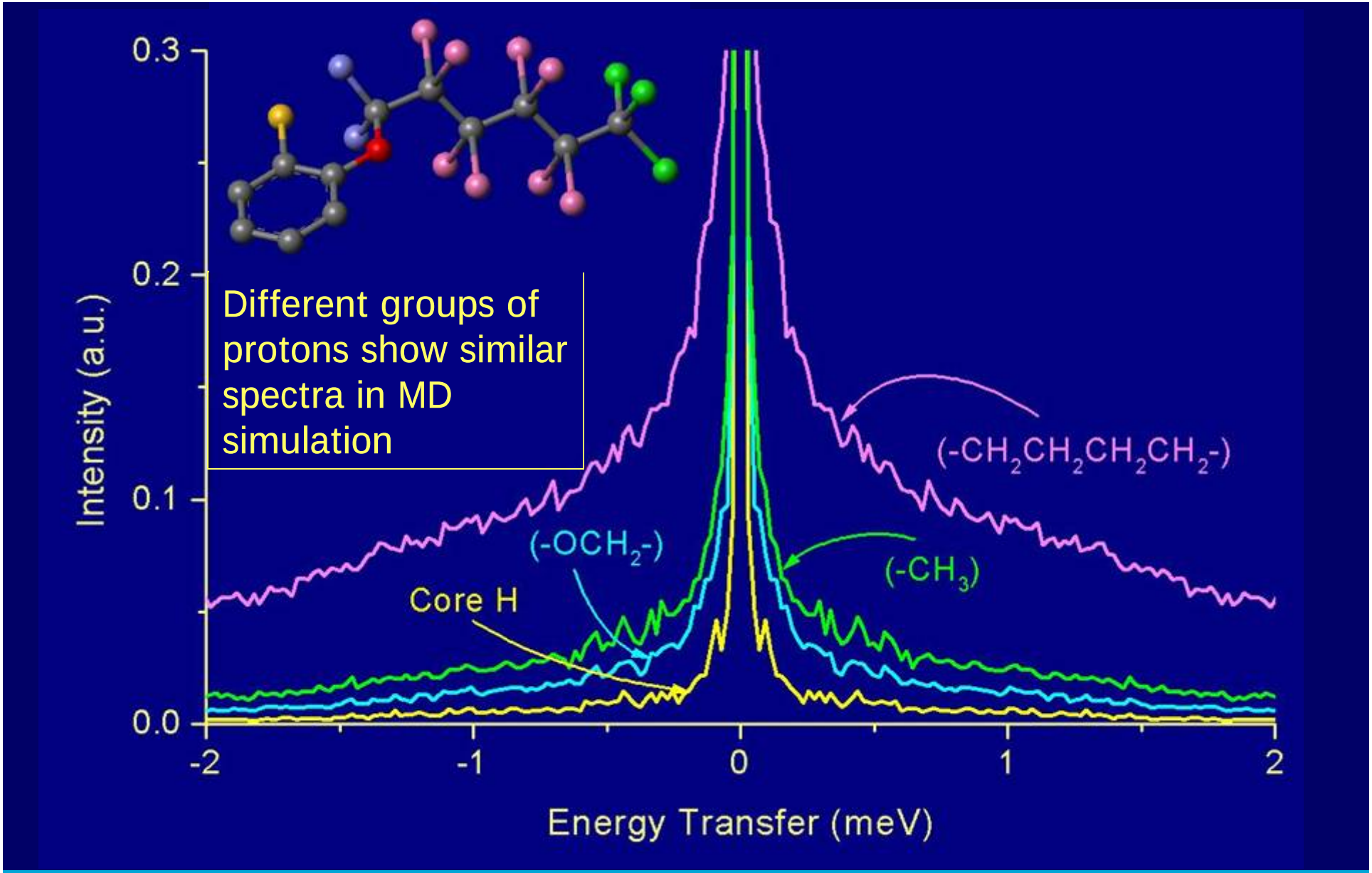
Force field molecular dynamics simulation



Out-of-plane motion on 7ps time-scale



Greater mobility in-plane on 0.2ps time-scale



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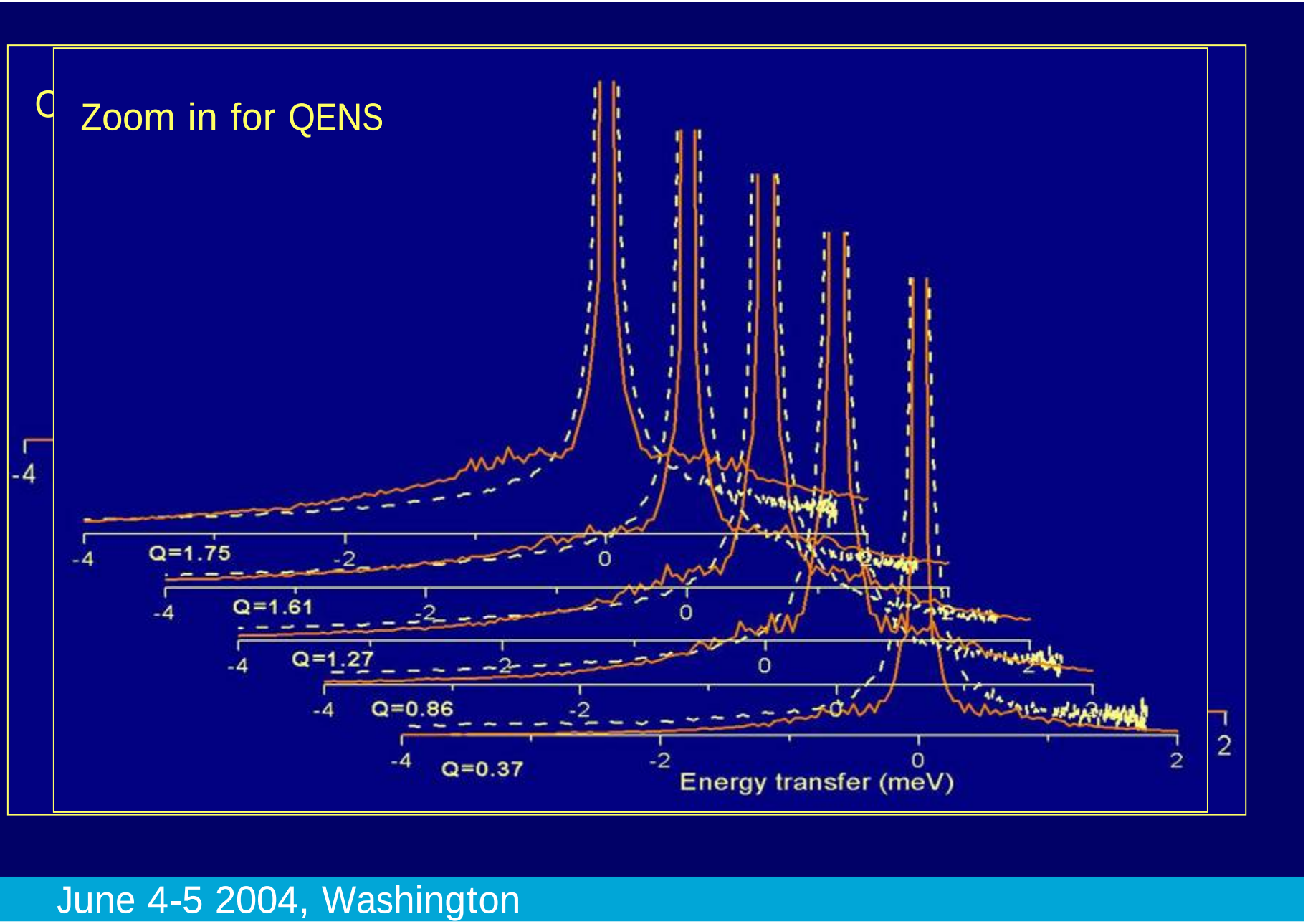

Zoom in for QENS
Q=1.75
Q=1.61
Q=1.27
Q=0.86
Q=0.37
Energy transfer (meV)

Force field molecular dynamics simulations suggest:

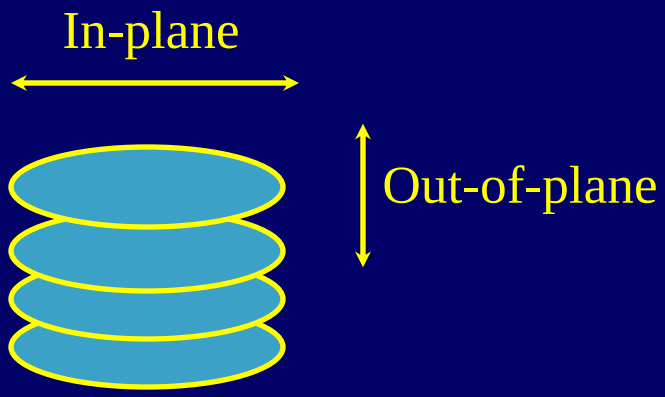
The experimentally observed motions could correspond to:

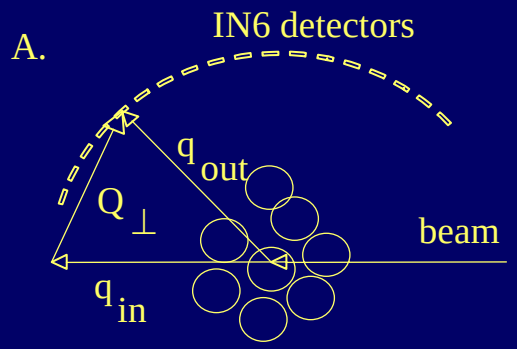
- Fast 7 ps motions:
  in plane
  amplitude: ~ 0.3 A

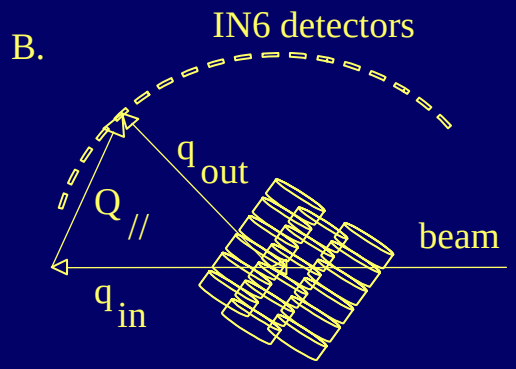
- Relatively slow 0.2 ps:
  out of plane motions
  amplitude: ~1.2A

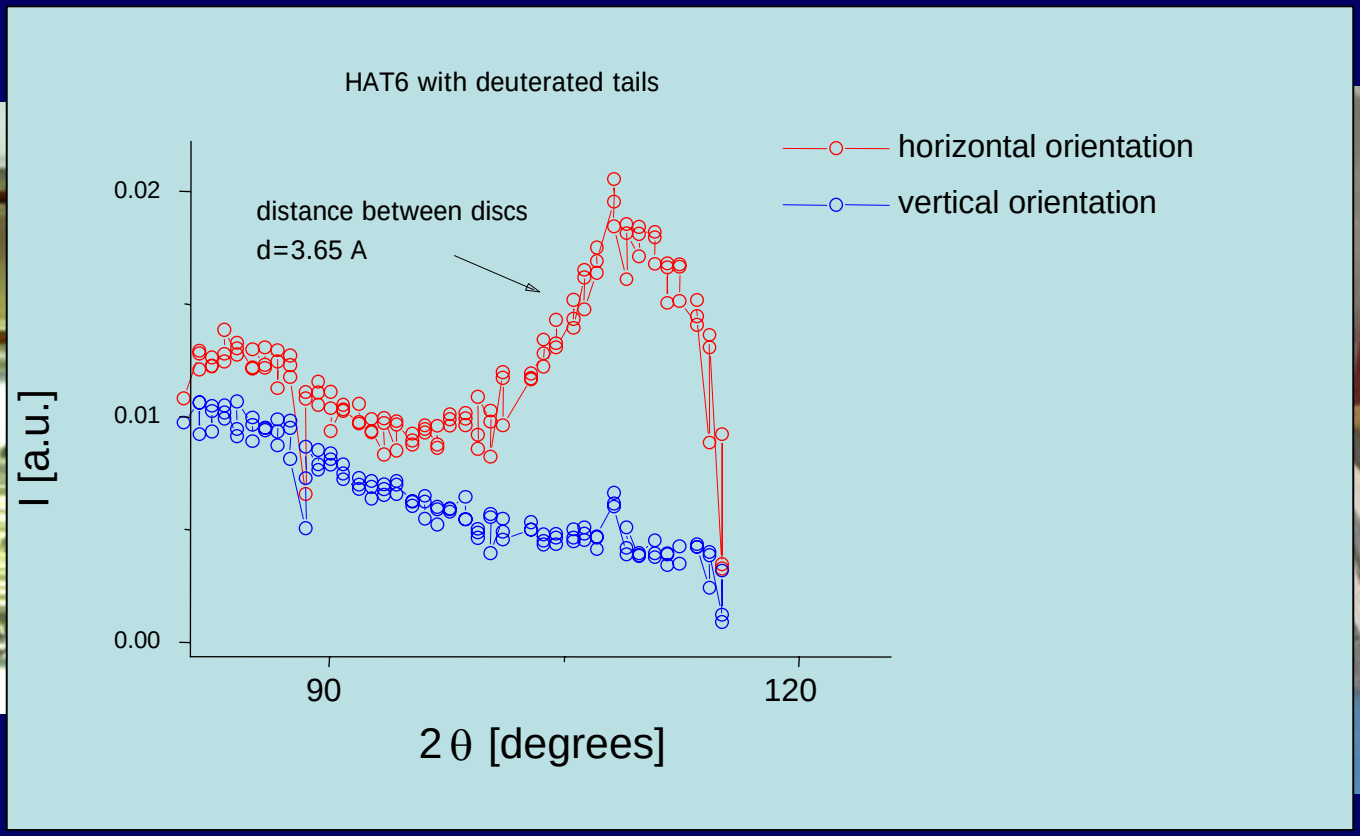
F.M. Mulder, *et al.* J. Am. Chem. Soc. 2003, 125, 3860-3866

Can one observe anisotropic dynamics?









Change in Bragg-peaks in quasi-elastic spectra shows orientation worked

Orient by shear at ~365K, then keep > 350K

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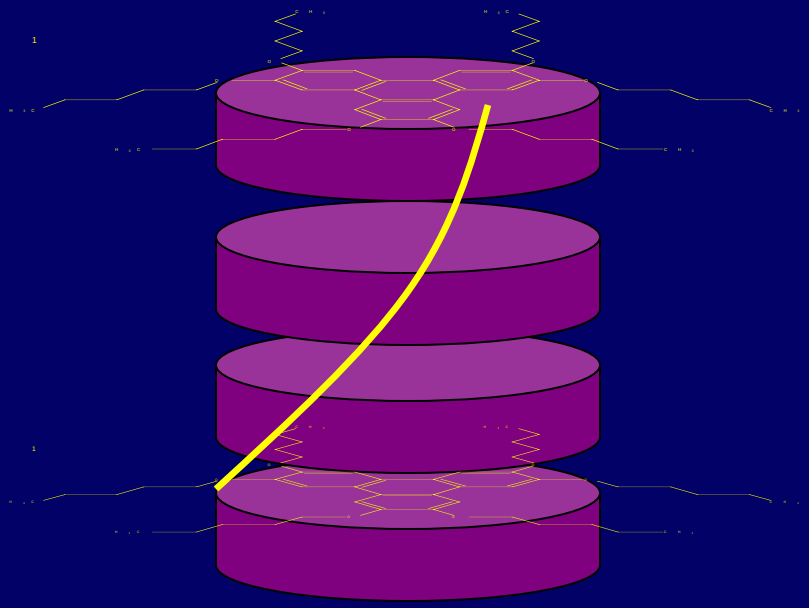
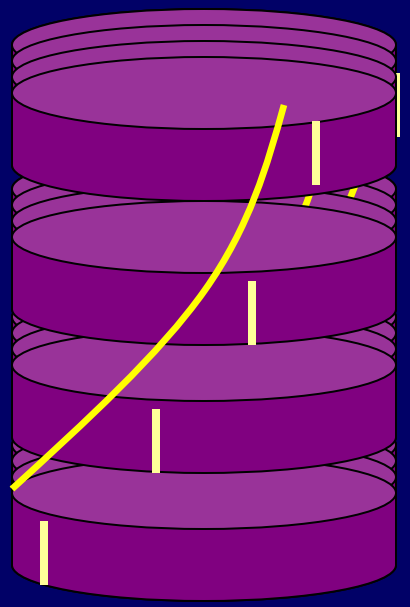
Result:

- not much difference between vertical and horizontal alignment

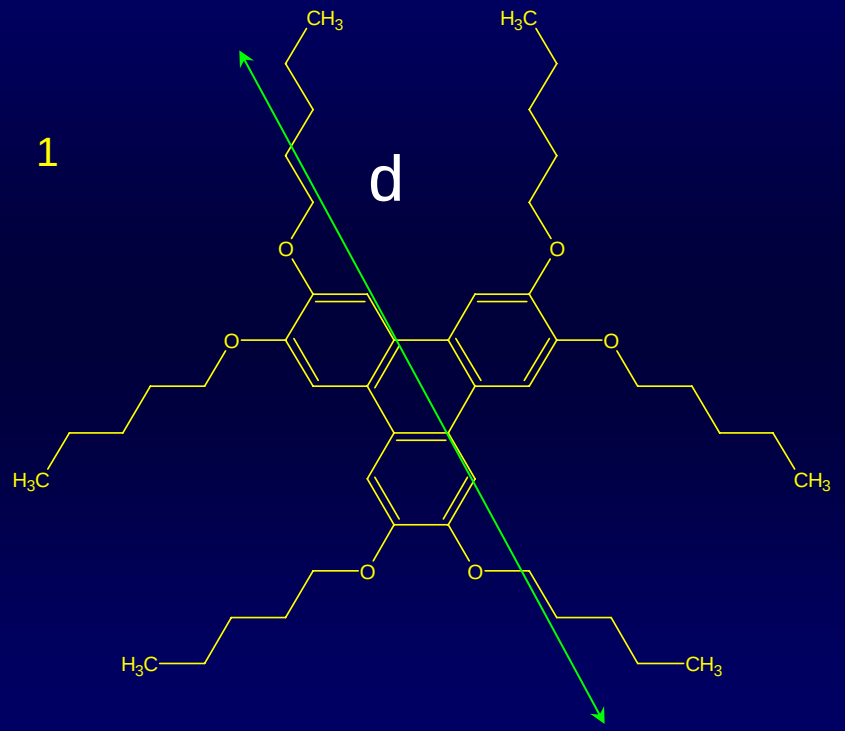
- both quasi elastic signals are still present

Helical modes would have
Similar amplitudes // and ⊥ to column





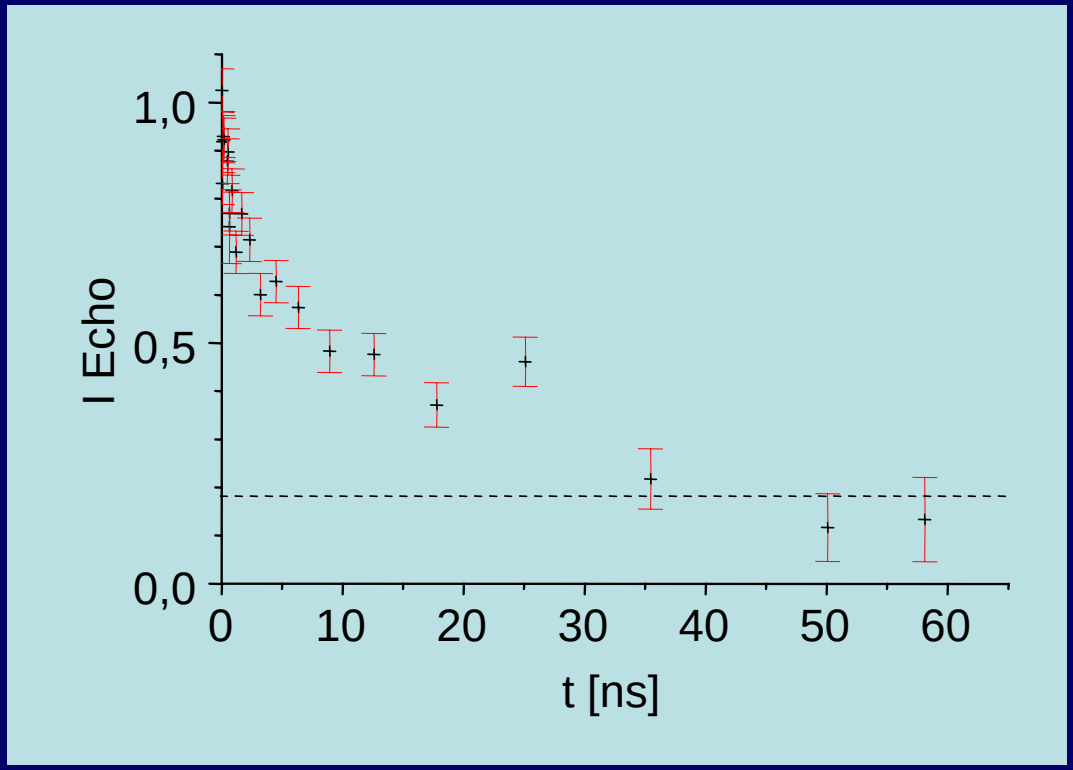
Relevant scale for the rotation of HAT6 molecule?



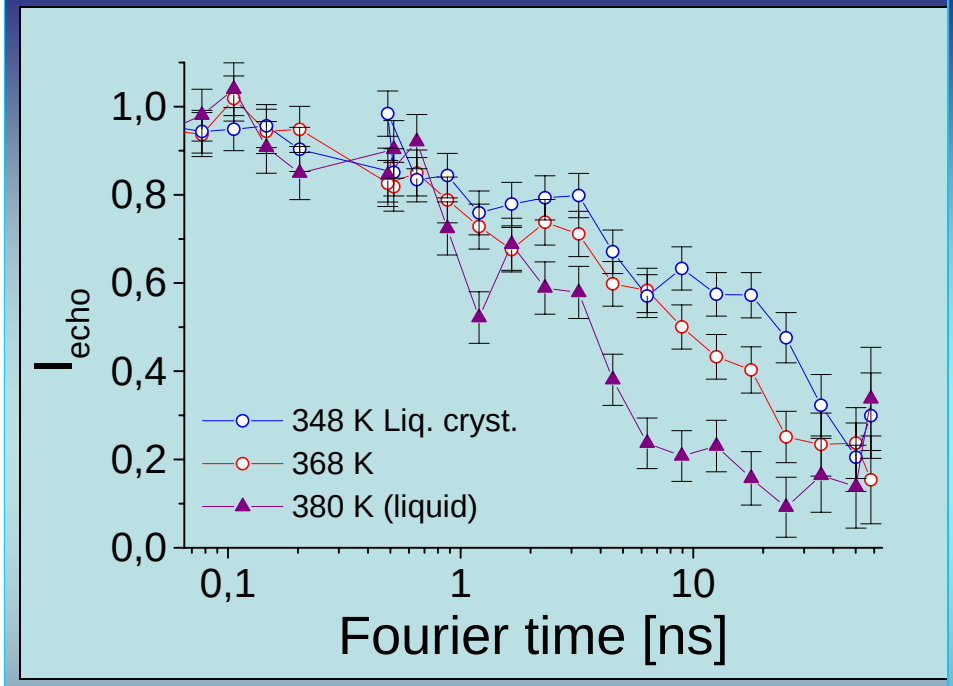
$$\frac{2\pi}{d} \sim 0.2\ \text{Å}^{-1}$$

Neutron Spin Echo

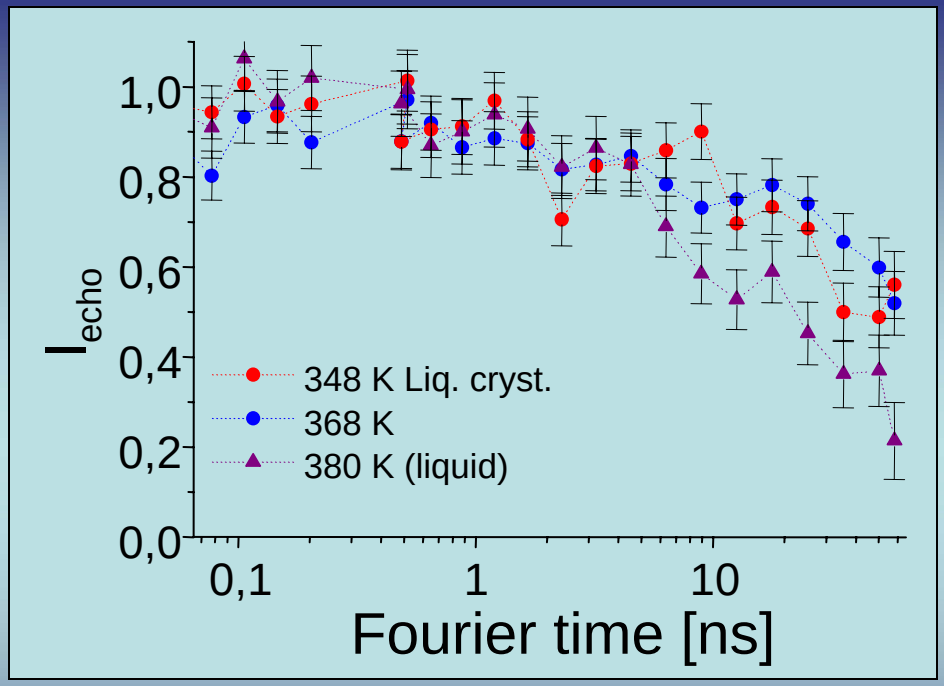
NSE (IN15, ILL Grenoble)



Limit for rotational diffusion

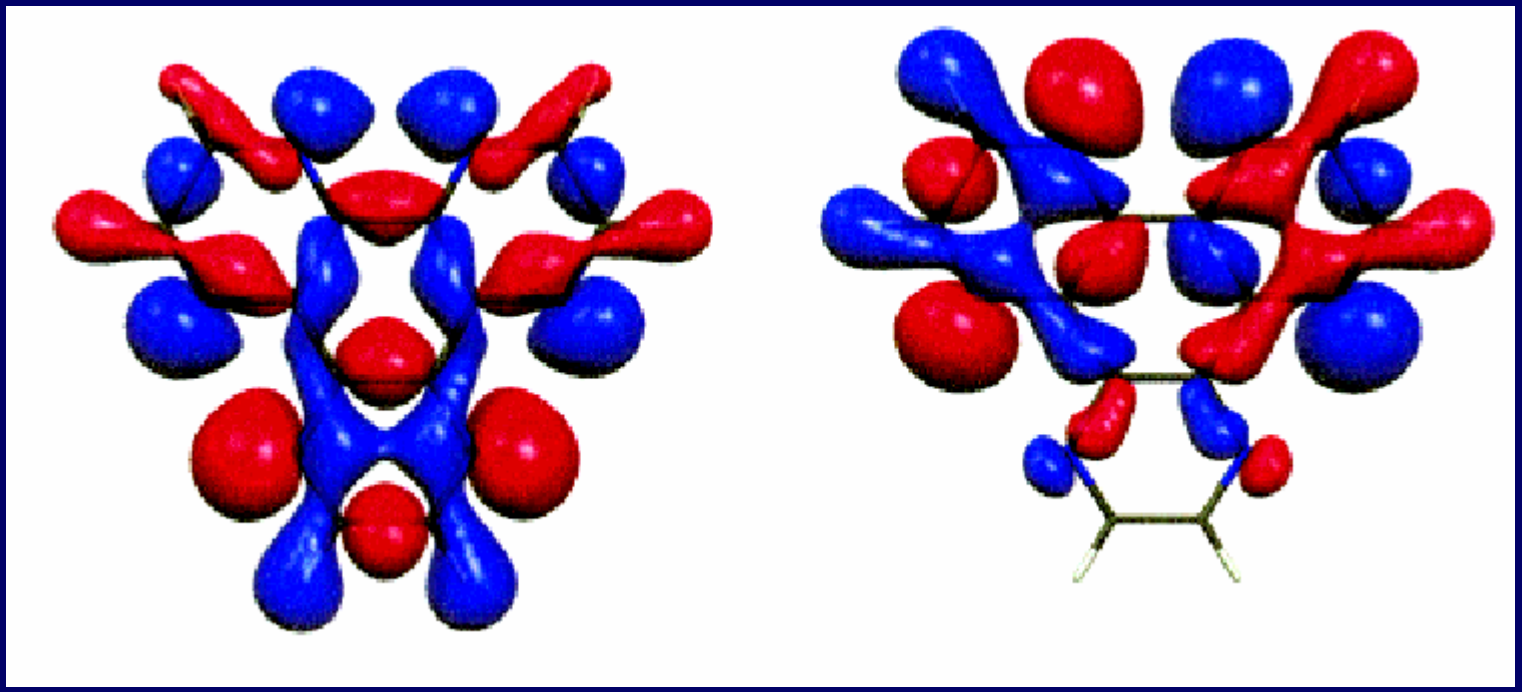

1,0
0,8
0,6
0,4
0,2
0,0
I echo
348 K Liq. cryst.
368 K
380 K (liquid)
0,1
1
10
Fourier time [ns]

Q = 0.2 Å^{-1}


1,0
0,8
0,6
0,4
0,2
0,0
I echo
348 K Liq. cryst.
368 K
380 K (liquid)
0,1
1
10
Fourier time [ns]

Q = 0.1 Å^{-1}

Conductivity?



First step: influence of certain vibrational modes on electronic orbitals

Conclusions

- neutron scattering combined with simulations yields structure & dynamics

- molecular and electronic dynamics have similar timescales in HAT6

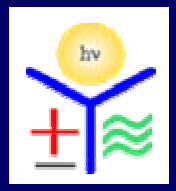
- simulations will yield conductivity, to be continued

‘Molecular dynamics assisted’ conductivity?

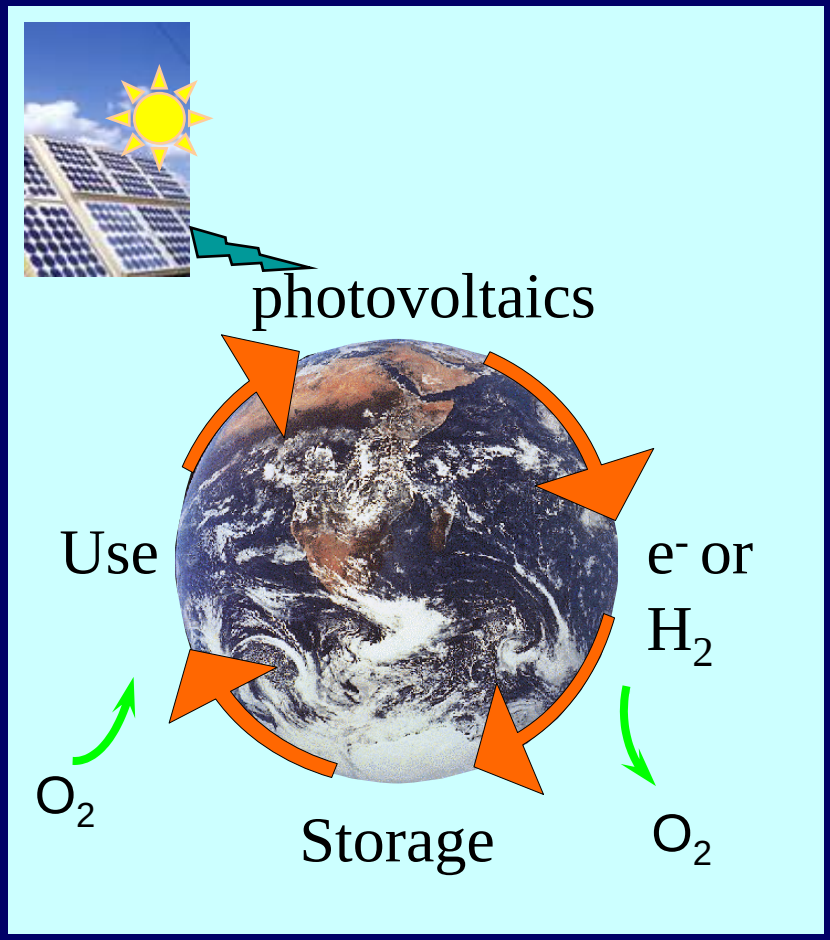
Acknowledgements

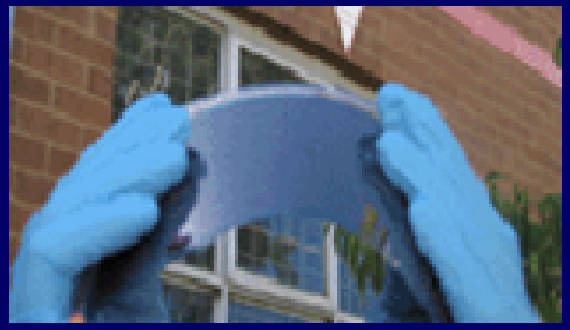
Dutch Science Foundation

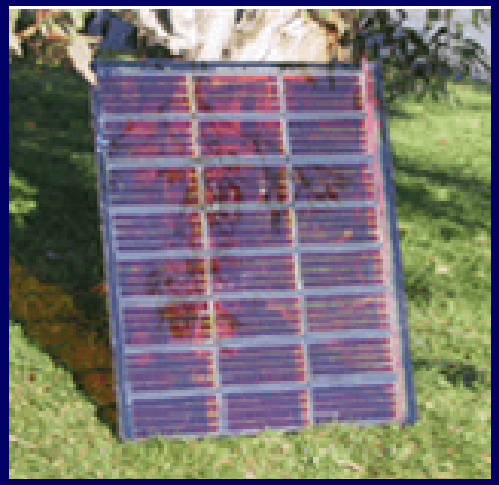
Chemical Sciences Foundation



Delft Institute for Sustainable Energy


photovoltaics
Use
e- or
H2
O2
Storage
O2





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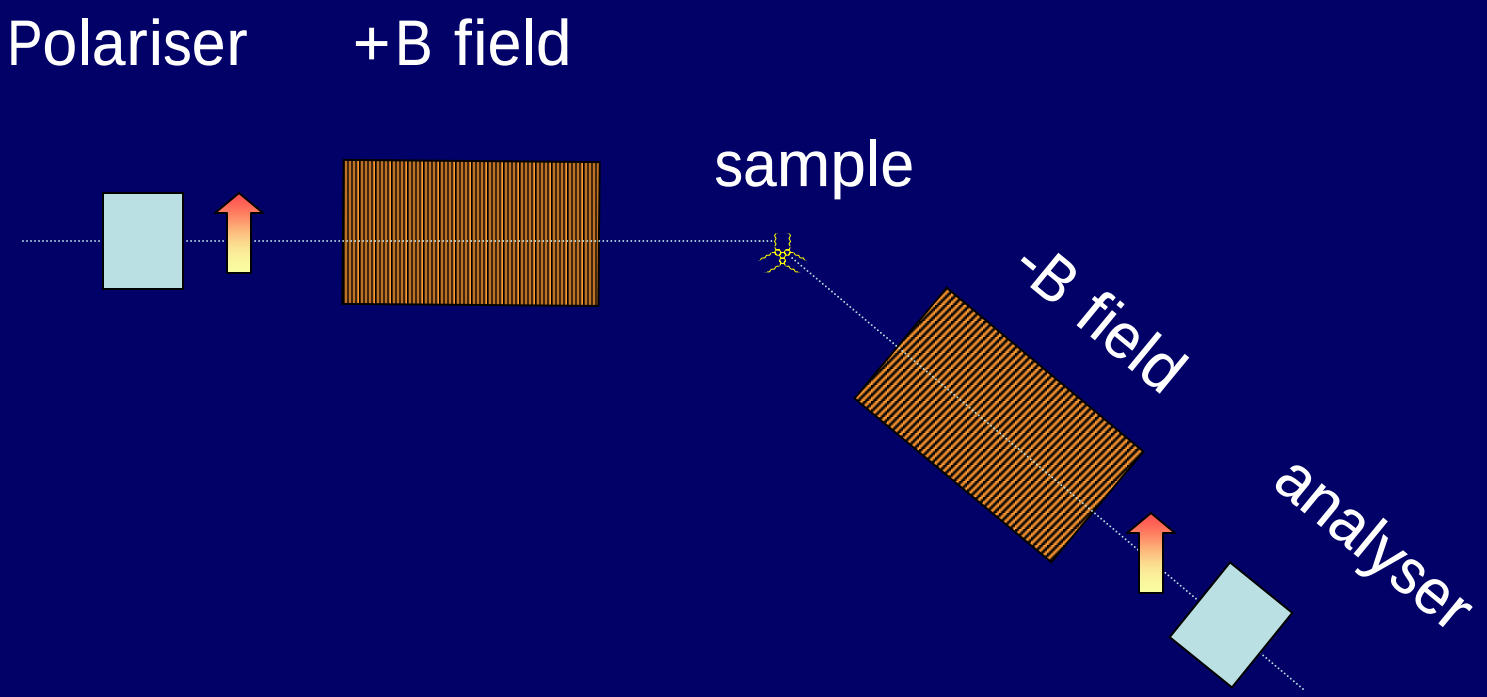
Slow dynamics of HAT6 observed by neutron spin echo



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